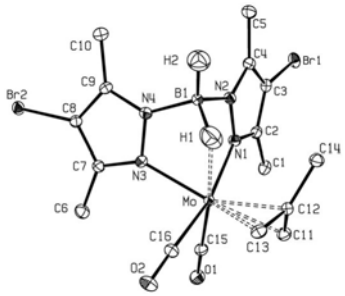
W0039

Crystal Neutron Diffraction Studies of 3-Center Agostic B—H—Mo Bonds. P.M.B. Piccoli, J.A. Cowan, T.F. Koetzle, A.J. Schultz, S. Trofimenko[†], IPNS, Argonne National Laboratory, Argonne, IL 60439, [†]Dept. of Chemistry, Univ. of Delaware, Newark, DE 19716.

The scorpionates, or polypyrazolylborate ligands, are the basis of rich coordination chemistry, and close to 180 scorpionates are now known. Over 30 years ago, agostic B—H—Mo 3-center bonds were found in scorpionates of the type H_2B(pyrazol-1-yl)$Mo(CO)_2$(L) where L = π-methylallyl. The first x-ray structure showing such a bond was reported in 1971 for [Bp*]$Mo(CO)_2$(π-allyl), Bp* = H_2B(3,5-dimethylpyrazol-1-yl), where the location of the bridging hydrogen was based on idealized approximations. In order to locate the bridging hydrogen with the precision that neutron diffraction data can provide and to assess the validity of the approximations for the location of agostic hydrogen atoms, single crystal diffraction data were collected at the Argonne Intense Pulsed Neutron Source (IPNS) on three scorpionates: [Bp^{Phe2}]$Mo(CO)_2$(L) (1), [Bp^{Me3}]$Mo(CO)_2$(L) (2) and [Bp^{*Br}]$Mo(CO)_2$(L) (3, see figure). Results show a lengthening of the B—H bond due to the bonding interaction with the metal. The effects of steric or electronic factors caused by varying substituents on the Bp ligands will be explored.



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